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Dear Bolko,

This is the third quarterly report of our second year in the Thin Film Partnership Program (Subcontract No. XXL-5-44205-12 to University of Nevada, Las Vegas: Characterization of the electronic and chemical structure at thin film solar cell interfaces). A brief summary and details of our activities are given below. This report is in fulfillment of the deliverable schedule of the subcontract statement of work (SOW).

Summary

This project is devoted to deriving the electronic structure of interfaces in $Cu(In,Ga)(S,Se)_2$ and CdTe thin film solar cells. By using a unique combination of spectroscopic methods (photoelectron spectroscopy, inverse photoemission, and X-ray absorption and emission) a comprehensive picture of the electronic (i.e., band alignment in the valence and conduction band) as well as chemical structure can be painted. The work focuses on (a) deriving the bench mark picture for world-record cells, (b) analyze state-of-the-art cells from industrial processes, and (c) aid in the troubleshooting of cells with substandard performance.

In the last months, we could complete our picture of the deeply buried chalcopyrite/back contact interface by continuing our experiments at the $Cu(In,Ga)Se_2$ ("CIGSe") and $Cu(In,Ga)(S,Se_2)$ ("CIGSSe")/back contact samples prepared by the group of W. Shafarman (Institute of Energy Conversion, University of Delaware). We find a pronounced chemical interaction between absorber and back contact, namely the formation of $MoSe_2$ (or $Mo(S,Se)_2$) and a diffusion of Ga into the Mo layer.

Detailed Description of the Activities:

In the past months we have continued our efforts of the characterization of the deeply buried interface between absorber and Mo back contact in chalcopyrite thin film solar cells. These investigations were based on two different types of samples, namely CIGSe/Mo/glass and CIGSSe/Mo/glass. Both sample types were provided by the group of W. Shafarman (IEC, U Delaware). In order to make the interface between absorber and Mo accessible for characterization by photoelectron spectroscopy (PES), we devel-

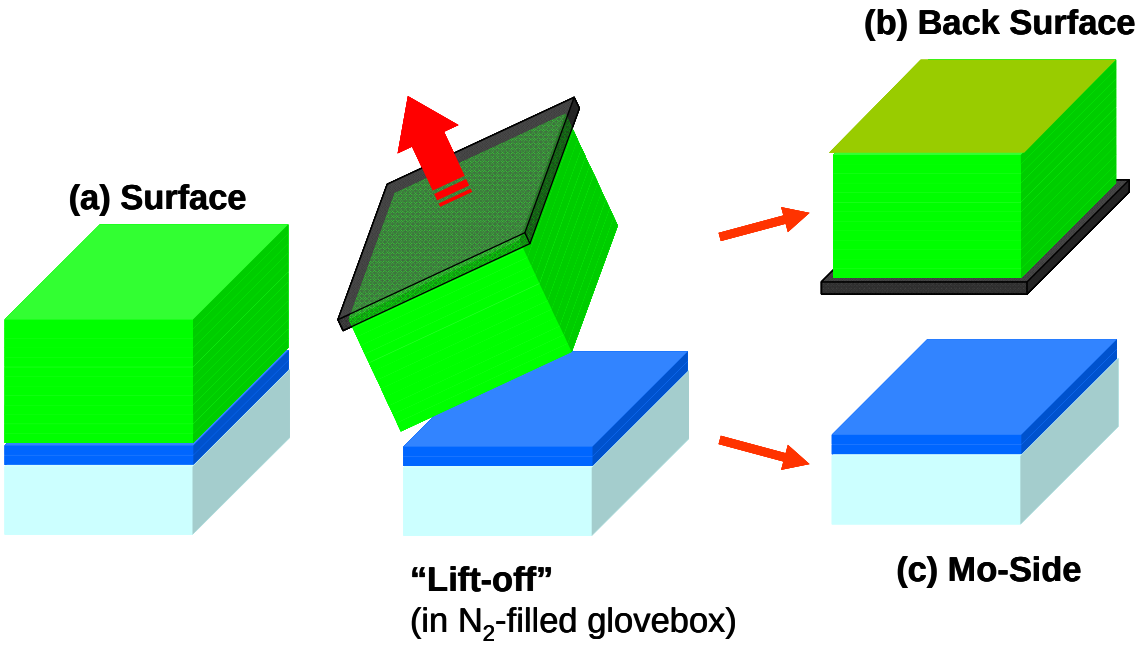

Fig. 1. *Scheme of the Lift-off process and visualization of the different prepared and investigated surfaces.*

oped a suitable lift-off (or cleavage) technique (as reported in our quarterly report in October 2006), which allowed us to cleave the absorber/Mo/glass samples at the desired interface. The scheme in Fig. 1 visualizes the different investigated surfaces for each lift-off process:

(a) Surface
(b) Back Surface
(c) Mo-Side

In this report we will focus on the results gained from the investigation of those samples by X-ray photoelectron spectroscopy (XPS). Fig. 2 shows the XPS survey spectra of the Surface, Back Surface, and Mo-Side of the CIGSSe (top) and CIGSe (bottom) samples. Although the samples were handled and shipped under inert gas atmosphere and stored in ultra-high vacuum (UHV), one can observe distinct peaks which can be ascribed to C and O on the Surface (a) stemming from a contamination layer formed on the absorber surface. In contrast, we find only minor amounts of C and O on the Back Surface (b). This shows that the applied cleavage process in a N_2 filled glovebag/glovebox and the immediate transfer of the cleaved samples into the attached UHV characterization system provides surfaces with minimized contamination.

The intensity difference of all absorber features (e.g., Ga 2p, Cu 2p, and In 3d) between Surface and Back Surface can be explained by the different attenuation of the differently thick contamination layers. Note that the C 1s signal observed on the Back Surface points to a C incorporation into the absorber layer. At first sight (see also discussion below) no Mo emission can be found on the Back Surface and only minor amounts of the absorber

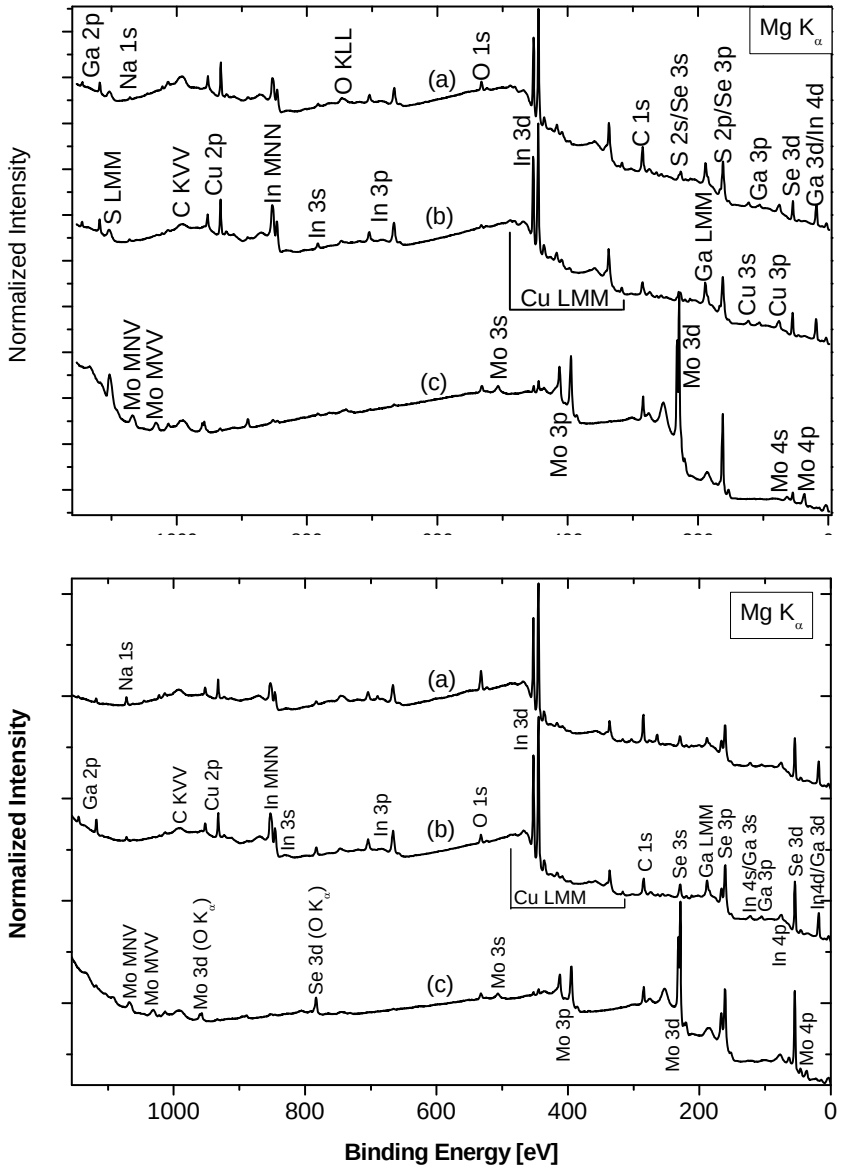

Fig. 2. *XPS survey spectra of the different accessible "surfaces" before and after lifting-off the chalcopyrite absorber from the Mo/glass substrate (top: CIGSSe, bottom: CIGSe): (a) Surface, (b) Back Surface, and (c)Mo-side.*

components (as indicated by the small In 3d peak - the most prominent absorber feature) can be observed on the Mo-Side. This confirms that the cleavage occurs at the absorber/Mo interface with only some chalcopyrite grains remaining on the back contact (this characteristic of the lift-off mechanism was already described in our Ref. [1]). In consequence, the comparatively large intensities of the photoemission and Auger lines of S and Se, respectively, observed on the Mo Front point to the formation of a $Mo(S,Se)_2$

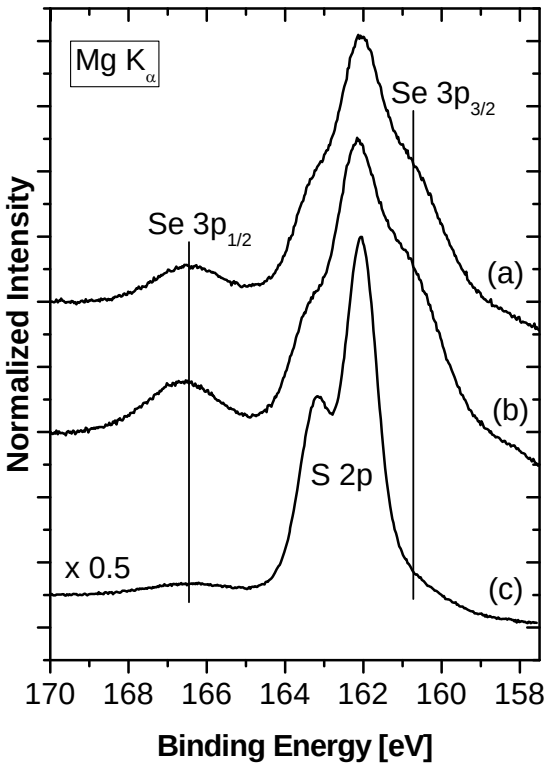

Fig. 3. *S 2p/ Se 3p photoemission of the different "surfaces" before and after lifting-off the CIGSSe absorber from the Mo/glass substrate: (a) Surface, (b) Back Surface, and (c)Mo-side.*

and $MoSe_2$ layer at the back contact for the CIGSSe and CIGSe sample. This was similarly reported/suggested in the past [1-7]. However, as shown in Fig. 3 (which shows the S 2p/Se 3p lines of the different CIGSSe-based samples), the S/Se ratio in the $Mo(S,Se)_2$ film does not mirror the S/Se ratio of the absorber. In this case, the formation of MoS_2 is clearly preferred over the formation of $MoSe_2$.

A more detailed analysis of our data indicates that (besides the formation of the $Mo(S,Se)_2$) additional chemical interactions at the absorber/back contact interface take place. A detailed comparison of the S 2s/Se 3s and Mo 3d energy range for the different samples (Surface, Back Surface, Mo-Side, Fig. 4) reveals that a (minor) Mo signal at the Back Surface can be identified at both absorber/back contact structures. This agrees with our earlier X-ray emission (XES) measurements [2] of different chalcopyrite/back contact structures, which also showed Mo at the absorber back side. It is at present unknown whether this is due to Mo diffusion into the Back Surface or the presence of some residual $Mo(S,Se)_2$ from the cleavage process.

A further result from the spectra in Fig. 4 is the finding that the $Mo(S,Se)_2$ layer (in the CIGSSe case) is apparently thinner than the $MoSe_2$ layer (in the CIGSe) case, as evidenced by the residual metallic Mo 3d doublet (filled black in Fig. 4, bottom left).

Our previous XES data also showed an accumulation/diffusion of Ga at/into the back contact [2]. Comparing the intensity of the most prominent photoemission lines of the absorber constituents Ga $2p_{3/2}$, Cu $2p_{3/2}$, and In $3d_{3/2}$ of the Back Surface and the absorber

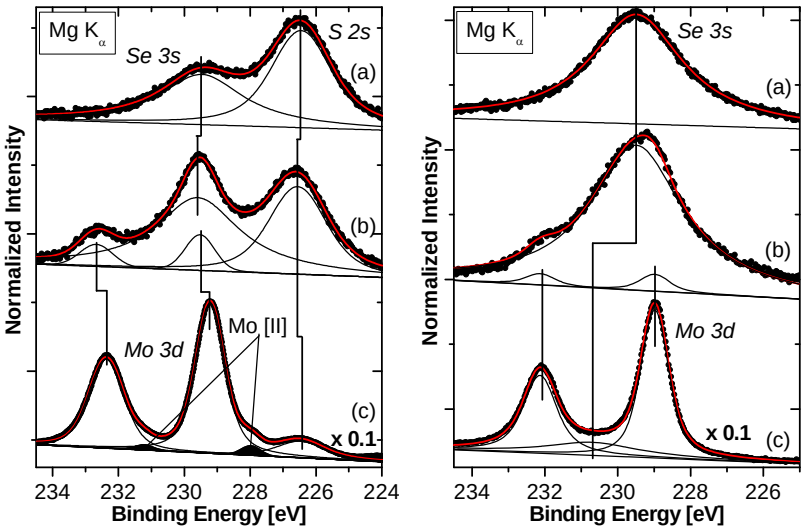

Fig. 4. *(Overlapping) S 2s/Se 3s and Mo 3d photoemission lines of the different "surfaces" before and after removing the chalcopyrite absorbers from the Mo/glass substrate (left: CIGSSe, right: CIGSe): (a) Surface, (b) Back Surface, and*

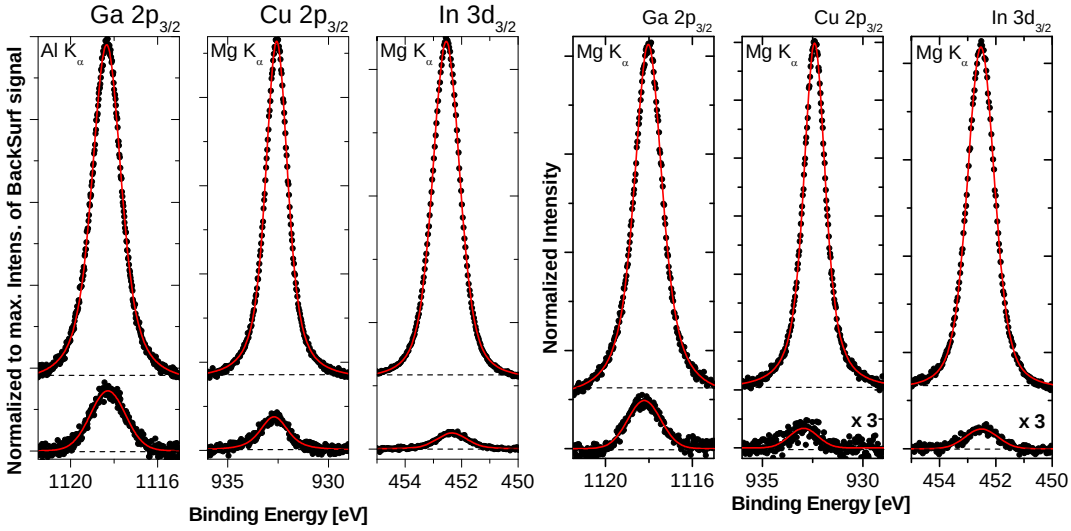

Fig. 5. *Comparison of the Ga 2p$_{3/2}$, Cu 2p$_{3/2}$, and In 3d$_{3/2}$ photoemission lines of the Back Surface (top) and absorber remainders at the Mo-Side (bottom). The intensities are normalized to the respective maximum of the Back Surface. CIGSSe (left) and CIGSe (right).*

remainders at the Mo-Side, our present XPS data confirms the accumulation of Ga. As shown in Fig. 5, we find that the Ga 2p intensity from the Mo-side is significantly larger than the intensity of the other absorber elements; note that the peaks in Fig. 5 were normalized to the absolute intensity of the respective peaks observed for the Back Surface, and hence a larger Ga peak directly indicates the presence of additional Ga on/in the Mo-side surface.

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If you have any questions, please do not hesitate to call me at (702) 895-2694.

Sincerely,

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